

L Number	Hits	Search Text	DB	Time stamp
-	62	gygi.in.	USPAT; US-PGPUB; EPO; JPO; DERWENT; IBM_TDB	2004/08/27 10:36
-	11	gygi.in. and steven.in.	USPAT; US-PGPUB; EPO; JPO; DERWENT; IBM_TDB	2004/08/27 10:36
-	22	("4798795"   "5240859"   "5438017"   "5514559"   "5527711"   "5534132"   "5534440"   "5538897"   "5614368"   "5650270"   "5658725"   "5686310"   "5738984"   "5851781"   "5863740"   "5880270"   "5952653"   "5958703"   "5965131"   "5965457"   "6017693"   "6057096").PN.	USPAT	2004/08/27 12:00
-	38	5538897.URPN.	USPAT	2004/08/27 12:13
-	1	"5240859".PN.	USPAT	2004/08/27 13:06
-	4	("5338686"   "5538897"   "5910403"   "6017693").PN.	USPAT	2004/08/27 13:06
-	22	("4798795"   "5240859"   "5438017"   "5514559"   "5527711"   "5534132"   "5534440"   "5538897"   "5614368"   "5650270"   "5658725"   "5686310"   "5738984"   "5851781"   "5863740"   "5880270"   "5952653"   "5958703"   "5965131"   "5965457"   "6017693"   "6057096").PN.	USPAT	2004/08/27 13:13
-	4	5910403.URPN.	USPAT	2004/08/27 13:18
-	2	("5338686"   "5439803").PN.	USPAT	2004/08/27 13:23
-	12	("Re33524"   "3959287"   "4022876"   "4224031"   "4732864"   "4866270"   "4952685"   "4957858"   "4970144"   "5059415"   "5084266"   "5124267").PN.	USPAT	2004/08/27 13:24
-	7	5338686.URPN.	USPAT	2004/08/27 13:36
-	15	("44647445"   "4656133"   "4830010"   "5059702"   "5317156"   "5386832"   "5413917"   "5439803"   "5542419"   "5837219"   "5910403"   "5916537"   "5924995"   "6010846"   "6355416").PN.	USPAT	2004/08/27 13:46
-	4	("5338686"   "5439803"   "5910403"   "6010846").PN.	USPAT	2004/08/27 13:50
-	1	6355416.URPN.	USPAT	2004/08/27 13:50
-	4	("5338686"   "5438194"   "5910403"   "6010846").PN.	USPAT	2004/08/27 13:51
-	17	4224031.URPN.	USPAT	2004/08/27 13:52
-	11	("4446237"   "4977320"   "5045694"   "5245186"   "5338686"   "5366721"   "5376355"   "5453247"   "5572024"   "5800979"   "6391649").PN.	USPAT	2004/08/27 14:14
-	1	6391649.URPN.	USPAT	2004/08/27 14:16
-	10	("4446237"   "4977320"   "5045694"   "5245186"   "5338686"   "5366721"   "5376355"   "5453247"   "5572024"   "5800979").PN.	USPAT	2004/08/27 14:16
-	3	6010846.URPN.	USPAT	2004/08/27 14:19
-	1	"5338686".PN.	USPAT	2004/08/27 14:19
-	11	5209919.URPN.	USPAT	2004/08/27 14:19
-	10	("3649199"   "4022876"   "4037100"   "4223004"   "4224031"   "4454233"   "4701419"   "5045479"   "5078135"   "5124267").PN.	USPAT	2004/08/27 14:22
-	1	"5209919".PN.	USPAT	2004/08/27 14:24
-	5	5376355.URPN.	USPAT	2004/08/27 14:24
-	1	"5209919".PN.	USPAT	2004/08/27 14:26
-	3	5366721.URPN.	USPAT	2004/08/27 14:26

-	189	( "3553452"   "3776700"   "3807235"   "3931516"   "4047030"   "4139346"   "4178359"   "4230797"   "4231999"   "4461328"   "4515781"   "4554839"   "4582789"   "4604363"   "4625112"   "4629689"   "4650750"   "4663944"   "4683195"   "4683202"   "4709016"   "4711955"   "4733073"   "4775619"   "4779467"   "4800159"   "4806546"   "4818681"   "4877745"   "4882127"   "4883750"   "4920264"   "4925629"   "4935357"   "4952518"   "5000921"   "5003059"   "5059654"   "5064754"   "5075217"   "5106585"   "5108703"   "5118605"   "5118937"   "5135870"   "5143451"   "5143854"   "5149625"   "5663242"   "5164594"   "5174962"   "5175209"   "5198540"   "5210412"   "5221518"   "5237016"   "5242974"   "5262128"   "5288644"   "5300774"   "5325021"   "5338688"   "5350676"   "5360819"   "5364759"   "5364760"   "5365063"   "5369004"   "5376355"   "5378602"   "5403711"   "5405746"   "5427929"   "5430136"   "5436143"   "5439649"   "5459039"   "5464985"   "5468610"   "5496562"   "5498545"   "5503980"   "5508169"   "5512295"   "5512439"   "5514548"   "5516931"   "5532227"   "5538897"   "5547835"   "5563410"   "5580434"   "5580733"   "5582979"   "5589136"   "5599500"   "5599666"   "5601982"   "5605662"   "5605798"   "5607912"   "5609907"   "5622824"   "5625184"   "5626184"   "5627369"   "5633496"   "5643800"   "5650489"   "5654150"   "5661028"   "5665967"   "5670322"   "5670381"   "5674686"   "5677195"   "5688642"   "5691141"   "5700642"   "5710028"   "5716825"   "5743960"   "5756050"   "5762876"   "5766847"   "5770367"   "5770860"   "5777324"   "5789395"   "5807522"   "5828063"   "5830655"   "5846717"   "5851765"   "5853989"   "5854486"   "5864137"   "5869240"   "5869242"   "5872003"   "5872010"   "5885775"   "5888819"   "5900481"   "5925520"   "5927547"   "5928906"   "5965363"   "5969350"   "5976798"   "5985356"   "5994065"   "6001567"   "6004744"   "6006171"   "6022688"   "6024925"   "6027890"   "6040193"   "6043031"   "6051378"   "6074823"   "6090558"   "6104028"   "6110426"   "6111251"   "6121048"   "6133436"   "6136269"   "6140045"   "6140053"   "6146854"   "6194144"   "6197498"   "6207370"   "6221601"   "6221605"   "6225061"   "6225450"   "6235478"   "6238871"   "6258538"   "6265716"   "6268131"   "6268144"   "6277573"   "6300076"   "6303309"   "6322970") . PN. (mass adj (spectroscopy spectrometry)) and subtractive	USPAT	2004/08/27 14:27
-	938	(mass adj (spectroscopy spectrometry)) and subtractive	USPAT; US-PGPUB; EPO; JPO; DERWENT; IBM TDB	2004/08/27 15:23

-	18	(mass adj (spectroscopy spectrometry)).ab,ti. and subtractive	USPAT; US-PGPUB; EPO; JPO; DERWENT; IBM TDB USPAT	2004/08/27 15:55
-	7	("5114551"   "5228960"   "5536382"   "5783397"   "6054047"   "6103537"   "6299747").PN.		2004/08/27 15:42
-	163	(mass adj (spectroscopy spectrometry)).ab,ti. and subtract\$	USPAT; US-PGPUB; EPO; JPO; DERWENT; IBM TDB USPAT;	2004/08/27 15:55
-	23	(mass adj (spectroscopy spectrometry)).ab,ti. and subtract\$.ab,ti.	USPAT; US-PGPUB; EPO; JPO; DERWENT; IBM TDB USPAT;	2004/08/27 15:56
-	15	("4314343"   "4524420"   "4546643"   "4802102"   "4837726"   "5092343"   "5291426"   "5592402"   "5633511"   "5737445"   "6047134"   "6112161"   "6147344"   "6178387"   "6266633").PN.	USPAT; US-PGPUB; EPO; JPO; DERWENT; IBM TDB USPAT	2004/08/27 16:00
-	7	6147344.URPN.	USPAT	2004/08/27 16:32
-	7	("5114551"   "5228960"   "5536382"   "5783397"   "6054047"   "6103537"   "6299747").PN.	USPAT	2004/08/27 16:40
-	12	inverse adj label\$	USPAT; US-PGPUB; EPO; JPO; DERWENT; IBM TDB	2004/08/30 12:42

L16 ANSWER 66 OF 71 BIOSIS COPYRIGHT (c) 2004 The Thomson Corporation. on  
STN

TI VARIATION OF NITROGEN-15 IN CORN AND SOIL FOLLOWING APPLICATION OF  
FERTILIZER NITROGEN.

L16 ANSWER 67 OF 71 BIOSIS COPYRIGHT (c) 2004 The Thomson Corporation. on  
STN

TI GAS CHROMATOGRAPHIC MASS SPECTROMETRIC ISOTOPE  
DILUTION DETERMINATION OF N N DI METHYL TRYPTAMINE CONCENTRATIONS IN  
NORMALS AND PSYCHIATRIC PATIENTS.

L16 ANSWER 68 OF 71 BIOSIS COPYRIGHT (c) 2004 The Thomson Corporation. on  
STN

TI GAS CHROMATOGRAPHIC MASS SPECTROMETRIC ISOTOPE  
DILUTION ASSAY FOR N N DI METHYL TRYPTAMINE IN HUMAN PLASMA.

L16 ANSWER 69 OF 71 BIOSIS COPYRIGHT (c) 2004 The Thomson Corporation. on  
STN

TI METABOLISM OF TRITIATED TESTOSTERONE BY THE ADRENAL OF THE DOG THE ACTION  
OF ACTH.

L16 ANSWER 70 OF 71 BIOSIS COPYRIGHT (c) 2004 The Thomson Corporation. on  
STN

TI SIMULTANEOUS MICRO ESTIMATION OF CHOLINE AND ACETYL CHOLINE BY GAS  
CHROMATOGRAPHY MASS SPECTROMETRY ISOTOPE  
DILUTION.

L16 ANSWER 71 OF 71 BIOSIS COPYRIGHT (c) 2004 The Thomson Corporation. on  
STN

TI A NEW METHOD OF PREPARING NITROGEN SAMPLES FROM HEME FOR MASS  
SPECTROMETRIC ISOTOPE ANALYSIS.

=> FIL CAPLUS		SINCE FILE	TOTAL
COST IN U.S. DOLLARS		ENTRY	SESSION
FULL ESTIMATED COST		16.95	58.25

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FILE COVERS 1907 - 30 Aug 2004 VOL 141 ISS 10  
FILE LAST UPDATED: 29 Aug 2004 (20040829/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> S (INVERSE (S) LABEL?)  
69666 INVERSE  
404642 LABEL?

L18 208 (INVERSE (S) LABEL?)

=> S (MASS (W) SPECTRO?)

821090 MASS

1273867 SPECTRO?

L19 224095 (MASS (W) SPECTRO?)

=> S (L18 (W) L19)

PROXIMITY OPERATOR LEVEL NOT CONSISTENT WITH

FIELD CODE - 'AND' OPERATOR ASSUMED 'L18 (W) L19'

L20 15 (L18 (W) L19)

=> DIS L20 1- TI

YOU HAVE REQUESTED DATA FROM 15 ANSWERS - CONTINUE? Y/ (N) :Y

THE ESTIMATED COST FOR THIS REQUEST IS 4.65 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:N

REQUEST CANCELED

=> DIS L20 1- TI

YOU HAVE REQUESTED DATA FROM 15 ANSWERS - CONTINUE? Y/ (N) :Y

THE ESTIMATED COST FOR THIS REQUEST IS 4.65 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:Y

L20 ANSWER 1 OF 15 CAPPLUS COPYRIGHT 2004 ACS on STN

TI **Inverse labeling** method for the rapid identification  
of marker/target proteins

L20 ANSWER 2 OF 15 CAPPLUS COPYRIGHT 2004 ACS on STN

TI **Inverse labeling-mass spectrometry**  
for the rapid identification of differentially expressed protein  
markers/targets

L20 ANSWER 3 OF 15 CAPPLUS COPYRIGHT 2004 ACS on STN

TI Biosynthesis of tunicamycin and metabolic origin of the 11-carbon dialdose  
sugar, tunicamine

L20 ANSWER 4 OF 15 CAPPLUS COPYRIGHT 2004 ACS on STN

TI **Inverse 15N-metabolic labeling/mass  
spectrometry** for comparative proteomics and rapid identification  
of protein markers/targets

L20 ANSWER 5 OF 15 CAPPLUS COPYRIGHT 2004 ACS on STN

TI **Inverse labeling** method for the rapid identification  
of marker/target proteins

L20 ANSWER 6 OF 15 CAPPLUS COPYRIGHT 2004 ACS on STN

TI **Inverse 18O labeling mass  
spectrometry** for the rapid identification of marker/target  
proteins

L20 ANSWER 7 OF 15 CAPPLUS COPYRIGHT 2004 ACS on STN

TI Nitrate contamination of drinking water: Relationship with HPRT variant  
frequency in lymphocyte DNA and urinary excretion of N-nitrosamines

L20 ANSWER 8 OF 15 CAPPLUS COPYRIGHT 2004 ACS on STN

TI Time-dependence of the isotope effects in the unimolecular dissociation of  
tertiary amine molecular ions

L20 ANSWER 9 OF 15 CAPPLUS COPYRIGHT 2004 ACS on STN

TI Development of a method for the determination of chlorpromazine and its  
major metabolites by gas chromatography/**mass  
spectrometry**, and application to biological fluids

L20 ANSWER 10 OF 15 CAPPLUS COPYRIGHT 2004 ACS on STN

TI Analysis of cholesterol, cholesterol-5,6-epoxides and cholestane-  
3 $\beta$ ,5 $\alpha$ ,6 $\beta$ -triol in nipple aspirates of human breast fluid  
by gas chromatography/**mass spectrometry**

L20 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN

TI Quantitation of serum bile acids by isotope dilution with  
carbon-13-labeled homologs

L20 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN

TI Determination of chlorpromazine and its major metabolites by gas  
chromatography/**mass spectrometry**: application to  
biological fluids

L20 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN

TI Biotransformation of mazindol. I. Isolation and identification of some  
metabolites from rat urine

L20 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN

TI Biosynthesis of streptomycin

L20 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN

TI **Mass spectrometry** in biochemical research

=> S (DUPLICATE (W) REMOVE)  
8920 DUPLICATE  
173338 REMOVE  
L21 0 (DUPLICATE (W) REMOVE)

=> d 120

L20 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 2004:451562 CAPLUS  
DN 141:20109  
TI **Inverse labeling** method for the rapid identification  
of marker/target proteins  
IN Wang, Yingqi Karen  
PA USA  
SO U.S. Pat. Appl. Publ., 63 pp., Cont.-in-part of U.S. Ser. No. 16,627.  
CODEN: USXXCO  
DT Patent  
LA English  
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2004106150	A1	20040603	US 2003-412964	20030414
	US 2002090652	A1	20020711	US 2001-16627	20011210
PRAI	US 2000-257559P	P	20001222		
	US 2001-332965P	P	20011119		
	US 2001-16627	A2	20011210		

=> d 120-  
L21 HAS NO ANSWERS  
L21 0 SEA FILE=CAPLUS (DUPLICATE (W) REMOVE)

=> d 120 1-  
YOU HAVE REQUESTED DATA FROM 15 ANSWERS - CONTINUE? Y/(N):Y

L20 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 2004:451562 CAPLUS  
DN 141:20109  
TI **Inverse labeling** method for the rapid identification

of marker/target proteins  
IN Wang, Yingqi Karen  
PA USA  
SO U.S. Pat. Appl. Publ., 63 pp., Cont.-in-part of U.S. Ser. No. 16,627.  
CODEN: USXXCO  
DT Patent  
LA English  
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2004106150	A1	20040603	US 2003-412964	20030414
	US 2002090652	A1	20020711	US 2001-16627	20011210
PRAI	US 2000-257559P	P	20001222		
	US 2001-332965P	P	20011119		
	US 2001-16627	A2	20011210		

L20 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 2003:41754 CAPLUS  
DN 138:350660  
TI **Inverse labeling-mass spectrometry**  
for the rapid identification of differentially expressed protein  
markers/targets  
AU Wang, Y. Karen; Quinn, Douglas F.; Ma, Zhixiang; Fu, Emil W.  
CS Central Technologies, Drug Discovery Research, Novartis Pharmaceuticals  
Corporation, Summit, NJ, 07901, USA  
SO Journal of Chromatography, B: Analytical Technologies in the Biomedical  
and Life Sciences (2002), 782(1-2), 291-306  
CODEN: JCBAAI; ISSN: 1570-0232  
PB Elsevier Science B.V.  
DT Journal  
LA English  
RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 2002:721474 CAPLUS  
DN 138:21926  
TI Biosynthesis of tunicamycin and metabolic origin of the 11-carbon dialdose  
sugar, tunicamine  
AU Tsvetanova, Billyana C.; Kiemle, David J.; Price, Neil P. J.  
CS Department of Chemistry, State University of New York, College of  
Environmental Science and Forestry, Syracuse, NY, 13210, USA  
SO Journal of Biological Chemistry (2002), 277(38), 35289-35296  
CODEN: JBCHA3; ISSN: 0021-9258  
PB American Society for Biochemistry and Molecular Biology  
DT Journal  
LA English  
RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 2002:557066 CAPLUS  
DN 137:228810  
TI **Inverse 15N-metabolic labeling/mass**  
**spectrometry** for comparative proteomics and rapid identification  
of protein markers/targets  
AU Wang, Y. Karen; Ma, Zhixiang; Quinn, Douglas F.; Fu, Emil W.  
CS Central Technologies, Discovery Research, Novartis Pharmaceuticals  
Corporation, Summit, NJ, 07901, USA  
SO Rapid Communications in Mass Spectrometry (2002), 16(14), 1389-1397  
CODEN: RCMSEF; ISSN: 0951-4198  
PB John Wiley & Sons Ltd.  
DT Journal  
LA English

RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 2002:505014 CAPLUS  
DN 137:59881  
TI **Inverse labeling** method for the rapid identification  
of marker/target proteins  
IN Wang, Yingqi Karen; Ma, Zhixiang; Quinn, Douglas Frederick; Fu, Emil W.  
PA Novartis A.-G., Switz.; Novartis-Erfindungen Verwaltungsgesellschaft  
m.b.H.  
SO PCT Int. Appl., 57 pp.  
CODEN: PIXXD2  
DT Patent  
LA English  
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002052271	A2	20020704	WO 2001-EP15228	20011221
	WO 2002052271	A3	20021031		
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LT, LU, LV, MA, MD, MK, MN, MX, NO, NZ, OM, PH, PL, PT, RO, RU, SE, SG, SI, SK, TJ, TM, TN, TR, TT, UA, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR			
	EP 1346229	A2	20030924	EP 2001-988064	20011221
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
	JP 2004516486	T2	20040603	JP 2002-553119	20011221
PRAI	US 2000-257559P	P	20001222		
	US 2001-332965P	P	20011119		
	WO 2001-EP15228	W	20011221		

L20 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 2001:484339 CAPLUS  
DN 135:119042  
TI **Inverse 18O labeling mass**  
**spectrometry** for the rapid identification of marker/target  
proteins  
AU Wang, Y. Karen; Ma, Zhixiang; Quinn, Douglas F.; Fu, Emil W.  
CS Core Technologies Area Discovery Research, Novartis Pharmaceuticals  
Corporation, Summit, NJ, 07901, USA  
SO Analytical Chemistry (2001), 73(15), 3742-3750  
CODEN: ANCHAM; ISSN: 0003-2700  
PB American Chemical Society  
DT Journal  
LA English  
RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 1996:438847 CAPLUS  
DN 125:95153  
TI Nitrate contamination of drinking water: Relationship with HPRT variant  
frequency in lymphocyte DNA and urinary excretion of N-nitrosamines  
AU Van Maanen, Jan M. S.; Welle, Irene J.; Hageman, Geja; Dallinga, Jan W.;  
Mertens, Paul L. J. M.; Kleinjans, Jos C. S.  
CS Department Health Risk Analysis and Toxicology, University Limburg,  
Maastricht, 6200 MD, Neth.  
SO Environmental Health Perspectives (1996), 104(5), 522-528  
CODEN: EVHPAZ; ISSN: 0091-6765

PB National Institute of Environmental Health Sciences  
DT Journal  
LA English

L20 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 1991:655477 CAPLUS  
DN 115:255477  
TI Time-dependence of the isotope effects in the unimolecular dissociation of tertiary amine molecular ions  
AU Ingemann, Steen; Kluft, Els; Nibbering, Nico M. M.; Allison, Colin E.; Derrick, Peter J.; Hammerum, Steen  
CS Inst. Mass Spectrom., Univ. Amsterdam, Amsterdam, 1018 WS, Neth.  
SO Organic Mass Spectrometry (1991), 26(10), 875-81  
CODEN: ORMSBG; ISSN: 0030-493X  
DT Journal  
LA English

L20 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 1988:400107 CAPLUS  
DN 109:107  
TI Development of a method for the determination of chlorpromazine and its major metabolites by gas chromatography/**mass spectrometry**, and application to biological fluids  
AU Craig, J. Cymerman; Gruenke, Larry D.; Klein, Frederick D.; Hitzemann, Barbara A.; Holaday, John W.; Loh, Horace H.; Braff, David L.; Fischer, Ames; Glick, Ira D.; et al.  
CS Dep. Chem. Pharm. Chem., Univ. California, San Francisco, CA, 94143, USA  
SO Neurology and Neurobiology (1988), 40(Perspect. Psychopharmacol.), 375-89  
CODEN: NEUND9; ISSN: 0736-4563  
DT Journal  
LA English

L20 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 1987:512049 CAPLUS  
DN 107:112049  
TI Analysis of cholesterol, cholesterol-5,6-epoxides and cholestan-3 $\beta$ ,5 $\alpha$ ,6 $\beta$ -triol in nipple aspirates of human breast fluid by gas chromatography/**mass spectrometry**  
AU Gruenke, L. D.; Craig, J. Cymerman; Petrakis, Nicholas L.; Lyon, Michael B.  
CS Sch. Pharm., Univ. California, San Francisco, CA, 94143, USA  
SO Biomedical & Environmental Mass Spectrometry (1987), 14(7), 335-8  
CODEN: BEMSEN; ISSN: 0887-6134  
DT Journal  
LA English

L20 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 1987:152498 CAPLUS  
DN 106:152498  
TI Quantitation of serum bile acids by isotope dilution with carbon-13-labeled homologs  
AU Stellaard, Frans; Paumgartner, Gustav  
CS Dep. Med. II, Univ. Munich, Munich, Fed. Rep. Ger.  
SO Clinica Chimica Acta (1987), 162(1), 45-51  
CODEN: CCATAR; ISSN: 0009-8981  
DT Journal  
LA English

L20 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 1986:141588 CAPLUS  
DN 104:141588  
TI Determination of chlorpromazine and its major metabolites by gas chromatography/**mass spectrometry**: application to biological fluids

AU Gruenke, L. D.; Craig, J. Cymerman; Klein, F. D.; Nguyen, T. L.; Hitzemann, Barbara A.; Holaday, J. W.; Loh, H. H.; Braff, L.; Fischer, Ames; et al.

CS Sch. Pharm., Univ. California, San Francisco, CA, 94143, USA

SO Biomedical Mass Spectrometry (1985), 12(12), 707-13

CODEN: BMSYAL; ISSN: 0306-042X

DT Journal

LA English

L20 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1976:471962 CAPLUS

DN 85:71962

TI Biotransformation of mazindol. I. Isolation and identification of some metabolites from rat urine

AU Dugger, Harry A.; Coombs, Renate A.; Schwarz, H. J.; Migdalof, Bruce H.; Orwig, Barbara A.

CS Drug Metab. Sect., Sandoz Pharm., East Hanover, NJ, USA

SO Drug Metabolism and Disposition (1976), 4(3), 262-8

CODEN: DMDSAI; ISSN: 0090-9556

DT Journal

LA English

L20 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1968:38112 CAPLUS

DN 68:38112

TI Biosynthesis of streptomycin

AU Tovarova, L.; Kornitskaya, E. Ya.; Pliner, S. A.; Puchkov, V. A.; Vul'fson, N. S.; Khokhlov, A. S.

CS Inst. Chem. Nat. Compounds, Acad. Sci. U.S.S.R., Moscow, USSR

SO Antibiot.; Adv. Res., Prod. Clin. Use, Proc. Congr. (1965), Meeting Date 1964, 604-7

CODEN: 16UDA2

DT Conference

LA English

L20 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1966:509883 CAPLUS

DN 65:109883

OREF 65:20500b-c

TI Mass spectrometry in biochemical research

AU Stenhagen, Einar

CS Univ. Goteborg, Swed.

SO Chimia (Aarau) (1966), 20(10), 346-57

DT Journal

LA English

=> FIL STNGUIDE

COST IN U.S. DOLLARS

SINCE FILE ENTRY	TOTAL SESSION
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FULL ESTIMATED COST

40.01	98.26
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COST IN U.S. DOLLARS

SINCE FILE ENTRY	TOTAL SESSION
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FULL ESTIMATED COST

0.30	98.56
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L24 ANSWER 1 OF 16 EMBASE COPYRIGHT 2004 ELSEVIER INC. ALL RIGHTS RESERVED.

on STN

ACCESSION NUMBER: 2004265778 EMBASE

TITLE: Peptide separations by slab gel electrophoresis in pluronic F127 polymer liquid crystals.

AUTHOR: Rill R.L.; Al-Sayah M.A.

CORPORATE SOURCE: R.L. Rill, Department of Biomedical Sciences, College of Medicine, Florida State University, Tallahassee, FL 32306-4300, United States. Randolph.Rill@med.fsu.edu

SOURCE: Electrophoresis, (2004) 25/9 (1249-1254).

Refs: 15

ISSN: 0173-0835 CODEN: ELCTDN

COUNTRY: Germany

DOCUMENT TYPE: Journal; Article

FILE SEGMENT: 029 Clinical Biochemistry

LANGUAGE: English

SUMMARY LANGUAGE: English

AB Proteomics and peptidomics could benefit from simple methods for high-resolution separation of oligopeptides analogous to slab gel electrophoresis of proteins. Gels of Pluronic F127 copolymer surfactant were investigated as media for slab gel electrophoresis of oligopeptides using a trypsin digest of myoglobin. Concentrated solutions of Pluronic F127 are fluid at low temperatures ( $\leq 5^{\circ}\text{C}$ ), but become a gel-like micellar liquid crystal upon warming. Nucleic acids are well separated by electrophoresis in these gels as previously shown by Rill and Liu. Good separations of myoglobin tryptic peptides were accomplished by electrophoresis on slab gels of 24% Pluronic F127 or 15% polyacrylamide using the alkaline Laemmli buffer system (without sodium dodecyl sulfate). Labeling of peptides with the succinimidyl ester of Cascade Yellow (CY) prior to electrophoresis allowed sensitive detection with blacklight illumination at 365 nm. Labeled tryptic peptides were identified by matrix-assisted laser desorption/ionization-time of flight (MALDI-TOF)-mass spectrometry. An inverse dependence of electrophoretic mobility on mass of peptides with charge Z = -1 was observed in both media. Two-dimensional (2-D) electrophoresis of myoglobin peptides on polyacrylamide, then on Pluronic media, at pH 8.3 indicated that the primary separation mechanism of most peptides was the same in both media. A few off-diagonal spots indicated that some peptides were preferentially retarded in Pluronic gels, perhaps due to hydrophobic effects. The ease of gel preparation and peptide recovery are advantages of Pluronic F127 gels for oligopeptide electrophoresis. The two media can be combined conveniently for 2-D electrophoresis, providing means to facilitate protein identification and peptidomics. .COPYRGT. 2004 Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim.

L24 ANSWER 2 OF 16 EMBASE COPYRIGHT 2004 ELSEVIER INC. ALL RIGHTS RESERVED.  
on STN

ACCESSION NUMBER: 2004189513 EMBASE

TITLE: Different structural states of the proteolipid membrane are produced by ligand binding to the human  $\delta$ -opioid receptor as shown by plasmon-waveguide resonance spectroscopy.

AUTHOR: Alves I.D.; Cowell S.M.; Salamon Z.; Devanathan S.; Tollin G.; Hruby V.J.

CORPORATE SOURCE: Dr. V.J. Hruby, Chemistry Department, University of Arizona, 1306 East University Boulevard, Tucson, AZ 85721, United States. hruby@u.arizona.edu

SOURCE: Molecular Pharmacology, (2004) 65/5 (1248-1257).

Refs: 45

ISSN: 0026-895X CODEN: MOPMA3

COUNTRY: United States

DOCUMENT TYPE: Journal; Article

FILE SEGMENT: 030 Pharmacology

037 Drug Literature Index

LANGUAGE: English  
SUMMARY LANGUAGE: English

AB Understanding structure-function relationships and mechanisms of signal transduction in G-protein-coupled receptors (GPCRs) is becoming increasingly important, both as a fundamental problem in membrane biology and as a consequence of their central role as pharmacological targets. Their integral membrane nature and rather low natural abundance present many challenging problems. Using a recently developed technique, plasmon-waveguide resonance (PWR) **spectroscopy**, we investigated the structural changes accompanying the binding of ligands to the human  $\delta$ -opioid receptor (hDOR) immobilized in a solid-supported lipid bilayer. This highly sensitive technique can directly monitor changes in mass density, conformation, and orientation occurring in such thin proteolipid films. Without requiring **labeling** protocols, PWR allows the direct determination of binding constants in a system very close to the receptor's natural environment. In the present study, conformational changes of a proteolipid membrane containing the hDOR were investigated upon binding of a variety of peptide and nonpeptide agonists, partial agonists, antagonists, and **inverse** agonists. Distinctly different structural states of the membrane were observed upon binding of each of these classes of ligands, reflecting different receptor conformational states, and the formation of each state was characterized by different kinetic properties. Binding constants, obtained by quantifying the extent of conformational change as a function of the amount of ligand bound, were in good agreement with published values determined by radiolabeling methods. The results provide new insights into ligand-induced GPCR functioning and illustrate a powerful new protocol for drug development.

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on STN

ACCESSION NUMBER: 2004126863 EMBASE

TITLE: Plasmon-Waveguide Resonance Studies of Ligand Binding to the Human  $\beta(2)$ -Adrenergic Receptor.

AUTHOR: Devanathan S.; Yao Z.; Salomon Z.; Kobilka B.; Tollin G.

CORPORATE SOURCE: G. Tollin, Dept. of Biochem./Molec. Biophys., University of Arizona, Tucson, AZ 85721, United States.  
gtollin@arizona.edu

SOURCE: Biochemistry, (23 Mar 2004) 43/11 (3280-3288).  
Refs: 34

COUNTRY: ISSN: 0006-2960 CODEN: BICHAW  
United States

DOCUMENT TYPE: Journal; Article

FILE SEGMENT: 029 Clinical Biochemistry  
037 Drug Literature Index

LANGUAGE: English

SUMMARY LANGUAGE: English

AB Plasmon-waveguide resonance (PWR) **spectroscopy** is an optical technique that can be used to probe the molecular interactions occurring within anisotropic proteolipid membranes in real time without requiring molecular **labeling**. This method directly monitors mass density, conformation, and molecular orientation changes occurring in such systems and allows determination of protein-ligand binding constants and binding kinetics. In the present study, PWR has been used to monitor the incorporation of the human  $\beta(2)$ -adrenergic receptor into a solid-supported egg phosphatidylcholine lipid bilayer and to follow the binding of full agonists (isoproterenol, epinephrine), a partial agonist (dobutamine), an antagonist (alprenolol), and an **inverse** agonist (ICI-118,551) to the receptor. The combination of differences in binding kinetics and the PWR spectral changes point to the occurrence of multiple conformations that are characteristic of the type of ligand, reflecting differences in the receptor structural states produced by the binding process. These results provide new evidence for the conformational heterogeneity of the liganded states formed by the  $\beta(2)$ -adrenergic

receptor.

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ACCESSION NUMBER: 2002434645 EMBASE  
TITLE: **Inverse labeling-mass spectrometry** for the rapid identification of differentially expressed protein markers/targets.  
AUTHOR: Wang Y.K.; Quinn D.F.; Ma Z.; Fu E.W.  
CORPORATE SOURCE: Y.K. Wang, Central Technologies, Drug Discovery Research, Novartis Pharmaceut. Corporation, 556 Morris Avenue, Summit, NJ 07901, United States.  
karen.wang@pharma.novartis.com  
SOURCE: Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, (25 Dec 2002) 782/1-2 (291-306).  
Refs: 11  
ISSN: 1570-0232 CODEN: JCBAAI  
PUBLISHER IDENT.: S 1570-0232(02)00561-5  
COUNTRY: Netherlands  
DOCUMENT TYPE: Journal; Article  
FILE SEGMENT: 029 Clinical Biochemistry  
LANGUAGE: English  
SUMMARY LANGUAGE: English  
AB Comparative proteomic studies can lead to the identification of protein markers for disease diagnostics and protein targets for potential disease interventions. An **inverse labeling** strategy based on the principle of protein stable isotope **labeling** and **mass spectrometric** detection has been successfully applied to three general protein **labeling** methods. In contrast to the conventional single experiment approach, two **labeling** experiments are performed in which the initial **labeling** is reversed in the second experiment. Signals from differentially expressed proteins will distinguish themselves by exhibiting a characteristic pattern of isotope intensity profile reversal that will lead to the rapid identification of these proteins. Application of the **inverse labeling** method is demonstrated using model systems for protein chemical **labeling**, protein proteolytic **labeling**, and protein metabolic **labeling**. The methodology has clear advantages which are illustrated in the various studies. The **inverse labeling** strategy permits quick focus on signals from differentially expressed proteins (markers/targets) and eliminates ambiguities caused by the dynamic range of detection. In addition, the **inverse labeling** approach enables the unambiguous detection of covalent changes of proteins responding to a perturbation.  
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ACCESSION NUMBER: 2002336591 EMBASE  
TITLE: Biosynthesis of tunicamycin and metabolic origin of the 11-carbon dialdose sugar, tunicamine.  
AUTHOR: Tsvetanova B.C.; Kiemle D.J.; Price N.P.J.  
CORPORATE SOURCE: N.P.J. Price, Dept. of Anesthesiology, University of Rochester, Box 711, 601 Elmwood Ave., Rochester, NY 14642-8711, United States. Neil\_Price@urmc.rochester.edu  
SOURCE: Journal of Biological Chemistry, (20 Sep 2002) 277/38 (35289-35296).  
Refs: 25  
ISSN: 0021-9258 CODEN: JBCHA3  
COUNTRY: United States  
DOCUMENT TYPE: Journal; Article  
FILE SEGMENT: 029 Clinical Biochemistry  
LANGUAGE: English

SUMMARY LANGUAGE: English

AB Tunicamycin is a reversible inhibitor of polyprenolphosphate: N-acetylhexosamine-1-phosphate translocases and is produced by several Streptomyces species. We have examined tunicamycin biosynthesis, an important but poorly characterized biosynthetic pathway. Biosynthetic precursors have been identified by incorporating radioactive and stable isotopes, and by determining the labeling pattern using electrospray ionization-collision induced dissociation-mass spectrometry (ESI-CID-MS), and proton, deuterium, and C-13 nuclear magnetic resonance (NMR) spectroscopy. Preparation and analysis of [uracil-5-(2)H]-labeled tunicamycin established the complete ESI-CID-MS fragmentation pathway for the major components of the tunicamycin complex. Competitive metabolic experiments indicate that 7 deuteriums incorporate into tunicamycin from [6,6'-(2)H,(2)H]-labeled D-glucose, 6 of which arise from D-GlcNAc and 1 from uridine and/or D-ribose. Inverse correlation NMR experiments (heteronuclear single-quantum coherence (HSQC)) of (13)C-labeled tunicamycin enriched from D-[1-(13)C] glucose suggest that the unique tunicamine 11-carbon dialdose sugar backbone arises from a 5-carbon furanose precursor derived from uridine and a 6-carbon N-acetylamino-pyranose precursor derived from UDP-D-N-acetylglucosamine. The equivalent incorporation of (13)C into both the  $\alpha$ -1" and  $\beta$ -1' anomeric carbons of tunicamycin supports a direct biosynthesis via 6-carbon metabolism. It also indicates that the tunicamine motif and the  $\alpha$ -1"-linked GlcNAc residue are both derived from the same metabolic pool of UDP-GlcNAc, without significant differential metabolic processing. A biosynthetic pathway is therefore proposed for tunicamycin for the first time: an initial formation of the 11-carbon tunicamine sugar motif from uridine and UDP-GlcNAc via uridine-5'-aldehyde and UDP-4-keto-6-ene-N-acetyl-hexosamine, respectively, and subsequent formation of the anomeric-to-anomeric  $\alpha$ ,  $\beta$ -1",11'-glycosidic bond.

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ACCESSION NUMBER: 2002276676 EMBASE

TITLE: Pharmacokinetics of plasma enfuvirtide after subcutaneous administration to patients with human immunodeficiency virus: Inverse Gaussian density absorption and 2-compartment disposition.

AUTHOR: Zhang X.; Nieforth K.; Lang J.-M.; Rouzier-Panis R.; Reynes J.; Dorr A.; Kolis S.; Stiles M.R.; Kinchelow T.; Patel I.H.

CORPORATE SOURCE: Dr. X. Zhang, Department of Clinical Pharmacology, Hoffmann-La Roche Inc., 340 Kingsland St, Nutley, NJ 07110, United States. xiaoping.zhang@roche.com

SOURCE: Clinical Pharmacology and Therapeutics, (2002) 72/1 (10-19).

Refs: 23

ISSN: 0009-9236 CODEN: CLPTAT

United States

COUNTRY: United States

DOCUMENT TYPE: Journal; Article

FILE SEGMENT: 004 Microbiology

030 Pharmacology

037 Drug Literature Index

LANGUAGE: English

SUMMARY LANGUAGE: English

AB Objective: Enfuvirtide (T-20) is the first of a novel class of human immunodeficiency virus (HIV) drugs that block gp41-mediated viral fusion to host cells. The objectives of this study were to develop a structural pharmacokinetic model that would adequately characterize the absorption and disposition of enfuvirtide pharmacokinetics after both intravenous and subcutaneous administration and to evaluate the dose proportionality of enfuvirtide pharmacokinetic parameters at a subcutaneous dose higher than

that currently used in phase III studies. Methods: Twelve patients with HIV infection received 4 single doses of enfuvirtide separated by a 1-week washout period in an open-label, randomized, 4-way crossover fashion. The doses studied were 90 mg (intravenous) and 45 mg, 90 mg, and 180 mg (subcutaneous). Serial blood samples were collected up to 48 hours after each dose. Plasma enfuvirtide concentrations were measured with use of a validated liquid chromatography-tandem mass spectrometry method. Results: Enfuvirtide plasma concentration-time data after subcutaneous administration were well described by an inverse Gaussian density function-input model linked to a 2-compartment open distribution model with first-order elimination from the central compartment. The model-derived mean pharmacokinetic parameters ( $\pm$ SD) were volume of distribution of the central compartment ( $3.8 \pm 0.8$  L), volume of distribution of the peripheral compartment ( $1.7 \pm 0.6$  L), total clearance ( $1.44 \pm 0.30$  L/h), intercompartmental distribution ( $2.3 \pm 1.1$  L/h), bioavailability ( $89\% \pm 11\%$ ), and mean absorption time (7.26 hours, 8.65 hours, and 9.79 hours for the 45-mg, 90-mg, and 180-mg dose groups, respectively). The terminal half-life increased from 3.46 to 4.35 hours for the subcutaneous dose range from 45 to 180 mg. Conclusions: An inverse Gaussian density function-input model linked to a 2-compartment open distribution model with first-order elimination from the central compartment was appropriate to describe complex absorption and disposition kinetics of enfuvirtide plasma concentration-time data after subcutaneous administration to patients with HIV infection. Enfuvirtide was nearly completely absorbed from subcutaneous depot, and pharmacokinetic parameters were linear up to a dose of 180 mg in this study.

L24 ANSWER 7 OF 16 EMBASE COPYRIGHT 2004 ELSEVIER INC. ALL RIGHTS RESERVED.  
on STN

ACCESSION NUMBER: 2001327504 EMBASE

TITLE: Inverse (<sup>18</sup>O labeling mass

spectrometry for the rapid identification of marker/target proteins.

AUTHOR: Wang Y.K.; Ma Z.; Quinn D.F.; Fu E.W.

CORPORATE SOURCE: Y.K. Wang, Core Technologies Area, Discovery Research, Novartis Pharmaceuticals Corporation, 556 Morris Avenue, Summit, NJ 07901, United States.

Karen.wang@pharma.novartis.com

SOURCE: Analytical Chemistry, (1 Aug 2001) 73/15 (3742-3750).

Refs: 25

ISSN: 0003-2700 CODEN: ANCHAM

COUNTRY: United States

DOCUMENT TYPE: Journal; Article

FILE SEGMENT: 029 Clinical Biochemistry

LANGUAGE: English

SUMMARY LANGUAGE: English

AB Systematic analysis of proteins is essential in understanding human diseases and their clinical treatments. To achieve the rapid and unambiguous identification of marker or target proteins, a new procedure termed "inverse labeling" is proposed. With this procedure, to evaluate protein expression of a diseased or a drug-treated sample in comparison with a control sample, two converse labeling experiments are performed in parallel. The perturbed sample (by disease or by drug treatment) is labeled in one experiment, whereas the control is labeled in the second experiment. When mixed and analyzed with its unlabeled counterpart for differential comparison using mass spectrometry, a characteristic inverse labeling pattern of mass shift will be observed between the two parallel analyses for proteins that are differentially expressed. In this study, protein labeling is achieved through (<sup>18</sup>O) incorporation into peptides by proteolysis performed in [(<sup>18</sup>O)]water. Once the peptides are identified with the characteristic inverse labeling pattern of (<sup>18</sup>O)/(<sup>16</sup>O) ion intensity shift, MS data of

peptide fingerprints or peptide sequence information can be used to search a protein database for protein identification. The methodology has been applied successfully to two model systems in this study. It permits quick focus on the signals of differentially expressed proteins. It eliminates the detection ambiguities caused by the dynamic range of detection on proteins of extreme changes in expression. It enables the detection of protein modifications responding to perturbation. This strategy can also be extended to other protein-labeling methods, such as chemical or metabolic labeling, to realize the same benefits.

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ACCESSION NUMBER: 96200372 EMBASE  
DOCUMENT NUMBER: 1996200372  
TITLE: Nitrate contamination of drinking water: Relationship with HPRT variant frequency in lymphocyte DNA and urinary excretion of N-nitrosamines.  
AUTHOR: Van Maanen J.M.S.; Welle I.J.; Hageman G.; Dallinga J.W.; Mertens P.L.J.M.; Kleinjans J.C.S.  
CORPORATE SOURCE: Health Risk Analysis and Toxicology, University of Limburg, PO Box 616, 6200 MD Maastricht, Netherlands  
SOURCE: Environmental Health Perspectives, (1996) 104/5 (522-528).  
ISSN: 0091-6765 CODEN: EVHPAZ  
COUNTRY: United States  
DOCUMENT TYPE: Journal; Article  
FILE SEGMENT: 017 Public Health, Social Medicine and Epidemiology  
046 Environmental Health and Pollution Control  
LANGUAGE: English  
SUMMARY LANGUAGE: English

AB We studied peripheral lymphocyte HPRT variant frequency and endogenous nitrosation in human populations exposed to various nitrate levels in their drinking water. Four test populations of women volunteers were compared. Low and medium tap water nitrate exposure groups (14 and 21 subjects) were using public water supplies with nitrate levels of 0.02 and 17.5 mg/l, respectively. Medium and high well water nitrate exposure groups (6 and 9 subjects) were using private water wells with mean nitrate levels of 25 and 135 mg/l, respectively. Higher nitrate intake by drinking water consumption resulted in a dose-dependent increase in 24-hr urinary nitrate excretion and in increased salivary nitrate and nitrite levels. The mean log variant frequency of peripheral lymphocytes was significantly higher in the medium well water exposure group than in the low and medium tap water exposure groups. An inverse correlation between peripheral lymphocyte labeling index and nitrate concentration of drinking water was observed. Analysis of N-nitrosamine in the urine of 22 subjects by gas chromatography-mass spectrometry revealed the presence of N-nitrosopyrrolidine in 18 subjects. Analysis of the mutagenicity of well water samples showed that a small number of the well water samples were mutagenic in the Ames Salmonella typhimurium test after concentration over XAD-2 resin. In conclusion, consumption of drinking water, especially well water, with high nitrate levels can imply a genotoxic risk for humans as indicated by increased HPRT variant frequencies and by endogenous formation of carcinogenic N-nitroso compounds from nitrate-derived nitrite.

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ACCESSION NUMBER: 96128241 EMBASE  
DOCUMENT NUMBER: 1996128241  
TITLE: Proteinuria and plasma hexosugars in early-stage glomerulonephritis.  
AUTHOR: Pitkanen E.  
CORPORATE SOURCE: Department of Clinical Chemistry, University Hospital, Haartmaninkatu 4, FIN-00290 Helsinki, Finland  
SOURCE: Clinical Nephrology, (1996) 45/4 (226-229).

ISSN: 0301-0430 CODEN: CLNHBI  
COUNTRY: Germany  
DOCUMENT TYPE: Journal; Article  
FILE SEGMENT: 028 Urology and Nephrology  
029 Clinical Biochemistry  
LANGUAGE: English  
SUMMARY LANGUAGE: English  
AB Marked changes in the plasma concentration of several non-glucose monosaccharides have been detected among patients with end-stage renal disease. To find changes specific to renal disease and not caused by a failing urinary excretion, we studied the plasma monosaccharide concentration in patients with early-stage glomerulonephritis whose renal function was normal or only mildly compromised. Plasma mannose, fructose and 1,5-anhydroglucitol (1,5-AG) concentrations were measured using gas chromatography/mass spectrometry and isotope-labelled sugar standard additions. The daily urinary protein excretion was positively correlated with the plasma cholesterol ( $r = 0.785$ ), mannose ( $r = 0.550$ ), triglyceride ( $r = 0.531$ ) and fructose ( $r = 0.401$ ) concentrations, while the correlation with 1,5-AG ( $r = -0.581$ ) was inverse. The correlations were statistically significant. As previous studies have revealed a close positive correlation between the plasma mannose and glucose concentrations, we calculated the mannose/glucose concentration ratio to find out whether the increase in mannose concentration was or was not explained by ambient glucose. There was a strong correlation between the ratio and the urinary protein excretion ( $r = 0.704$ ). It is inferred that the metabolic syndrome associated with glomerulonephritis and characterised by hyperlipidemia also involves a derangement in mannose and 1,5-AG metabolism.

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ACCESSION NUMBER: 94219850 EMBASE  
DOCUMENT NUMBER: 1994219850  
TITLE: Comparison of stable isotopes and radioisotopes in the measurement of iron absorption in healthy women.  
AUTHOR: Barrett J.F.R.; Whittaker P.G.; Fenwick J.D.; Williams J.G.; Lind T.  
CORPORATE SOURCE: University Department of Obstetrics, Leazes Wing, Royal Victoria Infirmary, Newcastle-upon-Tyne NE1 4LP, United Kingdom  
SOURCE: Clinical Science, (1994) 87/1 (91-95).  
ISSN: 0143-5221 CODEN: CSCIAE  
COUNTRY: United Kingdom  
DOCUMENT TYPE: Journal; Article  
FILE SEGMENT: 010 Obstetrics and Gynecology  
023 Nuclear Medicine  
037 Drug Literature Index  
LANGUAGE: English  
SUMMARY LANGUAGE: English

AB 1. Stable isotope methods are being used to investigate the absorption of dietary iron. In order to be certain that this new methodology is accurate, we have compared results obtained using stable isotopes and inductively coupled plasma mass spectrometry with those determined using a radioisotope and whole body counting. 2. The stable isotope  $^{54}\text{Fe}$  (2.8 mg) was given to 10 healthy non-pregnant women. Six women received the isotope in aqueous form, and four took it with a meat meal. The  $^{54}\text{Fe}$  served as a carrier for 10 ng of the radioisotope  $^{59}\text{Fe}$ . An ampoule (200  $\mu\text{g}$ ) of the isotope  $^{57}\text{Fe}$  or  $^{58}\text{Fe}$  was then given intravenously, and in serum samples taken over the next 10h the ratios of the stable iron isotopes were measured by inductively coupled plasma mass spectrometry and the oral iron absorption was calculated. This was then compared with the results obtained by using a whole body counter to measure (on day 0 and day 14) the  $\gamma$ -activity emitted by the radioisotope. 3. The mean iron absorption measured by both

methods ranged from 8% to 45%. Measurement of the post-absorptive serum enrichment of the stable isotopes provided estimates of absorption from both aqueous and food iron which were similar to that yielded by whole body counting, the mean difference being -1.5% (95% confidence interval -5.2 to 2.1%). Absorption estimated by stable isotopes exhibited the same **inverse** relationship with the serum ferritin level (body iron stores) to that known to exist with whole body counting. Similar estimates of food iron absorption were obtained irrespective of the type of isotope used as an extrinsic **label**, implying that stable isotopes are as valid as radioisotopes in reflecting intrinsic food iron absorption. 4. This study validates the use of stable isotopes and post- absorption curves as a new and accurate technique in the measurement of iron absorption.

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ACCESSION NUMBER: 94013908 EMBASE  
DOCUMENT NUMBER: 1994013908  
TITLE: Structural characterization of gangliosides from resting and endotoxin- stimulated murine B lymphocytes.  
AUTHOR: Portner A.; Peter-Katalinic J.; Brade H.; Unland F.; Bunte Meyer H.; Muthing J.  
CORPORATE SOURCE: Institut fur Zellkulturtechnik, Postfach 10 01 31,33501 Bielefeld, Germany  
SOURCE: Biochemistry, (1993) 32/47 (12685-12693).  
ISSN: 0006-2960 CODEN: BICHAW  
COUNTRY: United States  
DOCUMENT TYPE: Journal; Article  
FILE SEGMENT: 002 Physiology  
029 Clinical Biochemistry  
LANGUAGE: English  
SUMMARY LANGUAGE: English

AB B lymphocytes from CBA/J mice were stimulated in splenocyte cultures for 72 h with various endotoxins. Bisphosphoryl lipid A from Escherichia coli had the highest stimulatory effect followed by LPS of Citrobacter freundii and Salmonella minnesota as measured by [<sup>3</sup>H]thymidine uptake. Gangliosides of stimulated B cells (metabolically **labeled** with D-[1-<sup>14</sup>C]galactose and D- [1-<sup>14</sup>C]glucosamine) and unlabeled gangliosides from resting B cells (prepared from spleens without stimulus) were analyzed by high-performance TLC, DEAE anion-exchange HPLC, and immunostaining procedures. Contents of ganglioside-derived sialic acids, quantified by HPLC as their fluorescent derivatives, decreased from stimulated to resident B lymphocytes in the following order: LPS S. minnesota > LPS C. freundii > bisphosphoryl lipid A E. coli > resting B cells. Gangliosides of resting B cells contained more N- glycolyl- than N-acetylneurameric acid, whereas **inverse** ratios were found in activated cells, indicating a shift from N-glycolyl- to N-acetylneurameric acid due to stimulation. Furthermore, a higher disialoganglioside content was characteristic for activated B cells. Fast atom bombardment **mass spectrometry** was performed with permethylated mono- and disialoganglioside fractions of LPS S. minnesota and LPS C. freundii stimulated B cells. Major gangliosides were G(M1a) and G(D1a) beside minute amounts of G(D1b). The structural heterogeneity in the gangliosides was caused by (a) N-substitution of the sialic acids with either acetyl or glycolyl groups, (b) variation in the long-chain base (sphingosine, sphinganine), and (c) substitution of the ceramide moiety by fatty acids of different chain length and degree of unsaturation (C(16:0), C(24:0,24:1)). In summary, these findings indicate the predominance of the G(M1a) pathway in murine B lymphocytes whereas G(M1b)- type gangliosides are preferentially expressed in T lymphocytes as well as macrophages.

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on STN  
ACCESSION NUMBER: 87072780 EMBASE

DOCUMENT NUMBER: 1987072780  
TITLE: Quantitation of serum bile acids by isotope dilution with 13C-labelled homologs.  
AUTHOR: Stellaard F.; Paumgartner G.  
CORPORATE SOURCE: Department of Medicine II, Klinikum Grosshadern, University of Munich, D-8000 Munich 70, Germany  
SOURCE: Clinica Chimica Acta, (1987) 162/1 (45-51).  
CODEN: CCATAR  
COUNTRY: Netherlands  
DOCUMENT TYPE: Journal  
FILE SEGMENT: 029 Clinical Biochemistry  
023 Nuclear Medicine  
LANGUAGE: English

AB Quantitation of individual bile acids in serum can be carried out with radioimmunoassays or with gas chromatography. The most specific measurements are obtained with combined gas chromatography/**mass spectrometry** employing stable isotope **labelled** bile acids as internal standards. So far only the use of deuterated internal standards has been described for this purpose. 24-13C-**labelled** bile acids have not been used since correction for the natural abundance of the 13C contribution has to be made. Furthermore, the maximal degree of labelling of 13C-**labelled** bile acids is about 90%. This requires additional correction for the percentage of unlabelled molecules. Using 13C-**labelled** bile acids as internal standards and adequate corrections for isotope interference we have measured individual serum bile acids in healthy volunteers by **inverse** isotope dilution with coefficient of variation (CV) values of 5.4-6.2% determined for the total procedure of sample preparation and analytical technique. In fasting serum of 15 healthy volunteers chenodeoxycholic acid averaged  $0.98 \pm SD 0.77 \mu\text{mol/l}$ , cholic acid  $0.49 \pm 0.39 \mu\text{mol/l}$  and deoxycholic acid  $1.07 \pm 0.68 \mu\text{mol/l}$ . Two hours postprandially these values increased to  $2.42 \pm 1.46 \mu\text{mol/l}$  for chenodeoxycholic acid,  $0.81 \pm 0.45 \mu\text{mol/l}$  for cholic acid and  $1.66 \pm 1.02 \mu\text{mol/l}$  for deoxycholic acid. These data agree well with those described in the literature obtained with deuterated internal standards. It may be concluded that 24-13C-**labelled** bile acids are suitable as internal standards for quantitation of serum bile acids, if corrections for isotope interferences are made.

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ACCESSION NUMBER: 86071833 EMBASE  
DOCUMENT NUMBER: 1986071833  
TITLE: Determination of chlorpromazine and its major metabolites by gas chromatography/**mass spectrometry**: Application to biological fluids.  
AUTHOR: Gruenke L.D.; Craig J.C.; Klein F.D.; et al.  
CORPORATE SOURCE: Department of Pharmaceutical Chemistry, School of Pharmacy, University of California, San Francisco, CA 94143, United States  
SOURCE: Biomedical Mass Spectrometry, (1985) 12/12 (707-713).  
CODEN: BMSYAL  
COUNTRY: United Kingdom  
DOCUMENT TYPE: Journal  
FILE SEGMENT: 037 Drug Literature Index  
029 Clinical Biochemistry  
LANGUAGE: English

AB A method for the quantitative determination of chlorpromazine and five of its major metabolites in a single sample of biological fluid in the ng/ml range has been developed utilizing gas chromatography/**mass spectrometry** with selected ion recording. The assay is highly specific and quantification is accomplished by an **inverse** stable isotope dilution technique, using deuterium-labeled variants of the compounds as internal standards. In this way the concentrations of

chlorpromazine and five of its major metabolites (the sulfoxide, the N-oxide, the monodemethylated, the didemethylated, and the 7-hydroxylated compounds) can be determined in biological fluids. Levels in humans have been measured both in plasma and in red blood cells and are compared to those found in related in vitro studies.

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ACCESSION NUMBER: 81030656 EMBASE  
DOCUMENT NUMBER: 1981030656  
TITLE: Study of theophylline metabolism in premature human newborns using stable isotope labelling.  
AUTHOR: Brazier J.L.; Ribon B.; Desage M.; Salle B.  
CORPORATE SOURCE: Dept. Chim. Anal. Pharmaceut., Fac. Pharm., 69373 Lyon Cedex 2, France  
SOURCE: Biomedical Mass Spectrometry, (1980) 7/5 (189-192).  
CODEN: BMSYAL  
COUNTRY: United Kingdom  
DOCUMENT TYPE: Journal  
FILE SEGMENT: 029 Clinical Biochemistry  
023 Nuclear Medicine  
007 Pediatrics and Pediatric Surgery  
037 Drug Literature Index  
015 Chest Diseases, Thoracic Surgery and Tuberculosis

LANGUAGE: English  
AB A new metabolic pathway of theophylline has been investigated in premature human newborns using the ion cluster technique of stable isotope labelling combined with gas chromatography mass spectrometry. Labelled caffeine, paraxanthine and theobromine have been found in plasma and urine of two preterm newborns receiving [1,3-15N], [12-13C]theophylline for the treatment of primitive apneas. Theophylline is converted to caffeine by N-7 methylation. In adults, the inverse process exists wherein caffeine is demethylated to give theophylline.

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ACCESSION NUMBER: 79221313 EMBASE  
DOCUMENT NUMBER: 1979221313  
TITLE: Biotransformation of mazindol. III. Comparison of metabolism in rat, dog, and man.  
AUTHOR: Dugger H.A.; Madrid V.O.; Talbot K.C.; et al.  
CORPORATE SOURCE: Drug Metab. Sect., Sandoz Pharmaceut., East Hanover, N.J. 07936, United States  
SOURCE: Drug Metabolism and Disposition, (1979) 7/3 (132-137).  
CODEN: DMDSAI  
COUNTRY: United States  
DOCUMENT TYPE: Journal  
FILE SEGMENT: 030 Pharmacology  
037 Drug Literature Index

LANGUAGE: English  
AB After administration of tritium-labeled mazindol (I) six to seven metabolites from rat, dog, and human urine were isolated by Amberlite XAD-2 extraction, DEAE-Sephadex chromatography, and preparative thin-layer chromatography and characterized by mass spectrometry. In addition, six mazindol-related substances present in trace quantities were also characterized by mass spectrometry. The major metabolite in all three species was 5-(p-chlorophenyl)-2,5-dihydro-5-hydroxy-3H-imidazo[2,1-a]isoindol-3-one (II). Also present, but in lesser amounts, in all three species were 5-(p-chlorophenyl)-2,5-dihydro-2,5-dihydroxy-3H-imidazo[2,1-a]isoindol-3-one (III), what is probably 3-(p-chlorophenyl)-2-glycyl-3-hydroxy-1-isoindolinone (IV), and a fourth metabolite of unknown structure (VII). 2-(p-Chlorobenzoyl)-N-2-(aminoethyl)benzamide (VI), a major urinary

metabolite in man, was characterized by **mass spectrometry**, synthesized, and quantitated by **inverse isotope dilution** in human urine (12.0% of the dose) and in dog (7.3% of the dose) and rat (0.64% of the dose) urine and feces. VI, as a conjugate, was also shown to be the most slowly excreted of the human metabolites with a half-life of ca. 5.25 days. The dog was the only one of the three species studied to excrete 3-(*p*-chlorophenyl)-3-hydroxy-1-oxoisindoline-2-acetic acid (IX). Rat urine contained no conjugated metabolites; II and VI were found as conjugates in human urine; only IV was found in the conjugate fraction from dog urine. The latter may have arisen by hydrolysis of II during workup.

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ACCESSION NUMBER: 77099374 EMBASE

DOCUMENT NUMBER: 1977099374

TITLE: Biotransformation of mazindol. I. Isolation and identification of some metabolites from rat urine.

AUTHOR: Dugger H.A.; Coombs R.A.; Schwartz H.J.; et al.

CORPORATE SOURCE: Drug Metab. Sect., Sandoz Pharmaceut., East Hanover, N.J. 07936, United States

SOURCE: Drug Metabolism and Disposition, (1976) 4/3 (262-268).

CODEN: DMDSAI

DOCUMENT TYPE: Journal

FILE SEGMENT: 037 Drug Literature Index

030 Pharmacology

LANGUAGE: English

AB Three metabolites of tritium labeled mazindol were isolated from rat urine by the **inverse** isotope dilution technique in which the labeled metabolites were synthesized by a second, smaller group of rats. These metabolites were isolated by Amberlite XAD 2 chromatography and silica gel column and preparative thin layer chromatography. The major metabolite (II) was shown by **mass spectrometry** of its trimethylsilyl derivative, NMR **spectroscopy**, and degradation studies to be 5 (*p* chlorophenyl) 2,5 dihydro 5 hydroxy 3H imidazol [2,1 a] isoindol 3 one. A comparison of its **mass spectrum** with that of an authentic sample prepared from 1 (*p* chlorophenyl) 3 ethoxy 1 methoxy 1H isoindole and glycine ethyl ester confirmed the assignment. Metabolite III was shown by its **mass spectrum**, NMR spectrum, degradation, and analogy with metabolite II to be 5 (*p* chlorophenyl) 2,5 dihydro 2,5 dihydroxy 3H imidazo [2,1 a] isoindol 3 one. Only a small amount of metabolite IV was isolated as an artifact, 3 (*p* chlorophenyl) 2 glycyl 3 methoxy 1 isoindolinone, as shown by its **mass spectrum** and degradation to 2 (*p* chlorobenzoyl) benzoic acid. The metabolite IV is believed to be the corresponding 3 hydroxy compound. Synthesis of IV by base catalyzed hydrolysis of metabolite II supports the structural assignment. In addition, the facile conversion of synthetic IV into the corresponding 3 methoxy derivative by acidic methanol was also observed.